Solve substrate concentration profile in a spherical gel (solution via the trial & error shooting method)
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Dimensional Form:

$$\frac{d^2 s}{dr^2} + \frac{2}{r}\cdot\frac{ds}{dr} = \frac{1}{D_e}\cdot v(s) \qquad \text{B.C.} \qquad s(R)=s_b \qquad \frac{d}{dr}s(0)=0$$

$$v(s) = \frac{v_m \cdot s}{K_m + s + K_i \cdot s^2}$$

Model parameters:

$v_m := 0.001\cdot gm\cdot liter^{-1}\cdot sec^{-1}$ $\quad K_m := 1\cdot gm\cdot liter^{-1}$ $\quad K_i := 10\cdot liter\cdot gm^{-1}$

$D_e := 10^{-5}\cdot cm^2\cdot sec^{-1}$ $\quad R := 0.7\cdot cm$ $\quad s_b := 1\cdot gm\cdot liter^{-1}$

Transform above equations in a DIMENSIONLESS form:

$$\frac{d^2 s}{dr^2} + \frac{2}{r}\cdot\frac{ds}{dr} = \phi^2\cdot v(s) \qquad \text{B.C.:} \qquad s(1)=1 \qquad \frac{ds(0)}{dr}=0$$

Dimensionless model parameters:

$\beta := \frac{K_m}{s_b}$ $\quad \Gamma := K_i\cdot\frac{s_b}{\beta}$ $\quad \phi := R\cdot\sqrt{\frac{v_m}{D_e\cdot K_m}}$

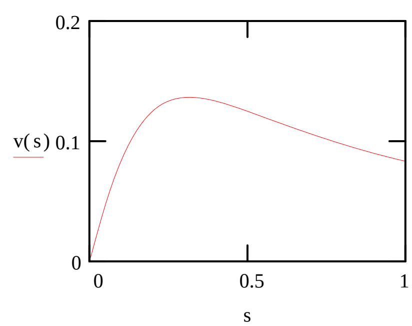
$\beta = 1$ $\quad \Gamma = 10$ $\quad \phi = 7$

Dimensionless model parameters and rate expression:

$\beta := 1$ $\quad \Gamma := 10$ $\quad \phi = 7$

$$v(s) := \frac{s}{1 + \frac{s}{\beta} + \Gamma\cdot s^2}$$

$s := 0, 0.01 .. 1$



Transform the above equation into two 1st-order ODEs:

$dsdr(r,s,z) := z$

$dzdr(r,s,z) := \phi^2\cdot v(s) - 2\cdot \text{if}\left(r=0, \frac{\phi^2}{3}\cdot v(s), \frac{z}{r}\right)$

$ODE(r,y) := \begin{pmatrix} dsdr(r, y_1, y_2) \\ dzdr(r, y_1, y_2) \end{pmatrix}$ With ORIGIN=1

Provide/guess initial values

$y_{initial} := \begin{pmatrix} 0.0805 \\ 0 \end{pmatrix}$ ← unknown value (guess this value until s(N)=1)
← known value

Integrate ODE

$N := 100 \quad i := 1 .. N$

$yout := rkfixed(y_{initial}, 0, 1, N, ODE)$

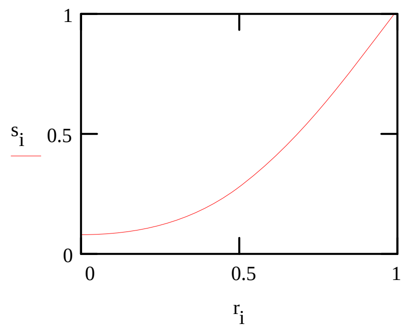
Use our own variable names

$r_i := yout_{i,1}$ $s_i := yout_{i,2}$ $dsdr_i := yout_{i,3}$

Values at r=1

$s_N = 1$ $dsdr_N = 1.769$

Plot of substrate profile



Compute the effectiveness factor, which is (observed rate / max rate without mass transfer limitation):

$$\eta := \frac{dsdr_N}{\frac{1}{3} \cdot \phi^2 \cdot v(1)} \qquad \eta = 1.299$$

In dimensional units, the reaction rate without mass transfer limitation is: $rate_m := \left(\frac{4}{3} \cdot \pi \cdot R^3\right) \cdot \left(\frac{v_m}{\beta} \cdot v(1)\right)$

which, is of course, the same as: $rate_m := \left(\frac{4}{3} \cdot \pi \cdot R^3\right) \cdot \left(\frac{v_m \cdot s_b}{K_m + s_b + K_i \cdot s_b^2}\right)$

observed rate = $\eta \cdot rate_m = 1.556 \cdot 10^{-7} \cdot gm \cdot sec^{-1}$

Alternative Solution of the Boundary Value Problem.

Trial-And-Error. We can define the solution of the ode as a function of the initial condition vector.

$$yout(y_{initial}) := rkfixed(y_{initial}, 0, 1, N, ODE)$$

The value of y_N at x=1 is a function of the initial condition vector.

$$s_N(y_{initial}) := rkfixed(y_{initial}, 0, 1, N, ODE)_{N,2}$$

$$s_N\left(\begin{pmatrix} 0.0805 \\ 0 \end{pmatrix}\right) = 1$$ ← guess $y_{initial}$ until the function gives 1

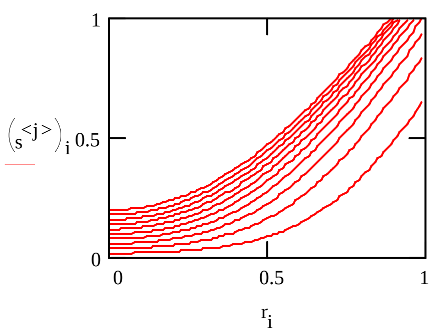
Since the second initial condition is set and there is no need to guess it, we can define a function which depends only on the initial condition that we need to guess to make the matter simpler.

$$yout(s_0) := rkfixed\left[\begin{pmatrix} s_0 \\ 0 \end{pmatrix}, 0, 1, N, ODE\right]$$

We shall generate a series of trajectories for different initial values. $j := 1 .. 10$ $\quad s_{0_j} := 0.02 \cdot j$

$$s^{<j>} := rkfixed\left[\begin{pmatrix} s_{0_j} \\ 0 \end{pmatrix}, 0, 1, N, ODE\right]^{<2>}$$

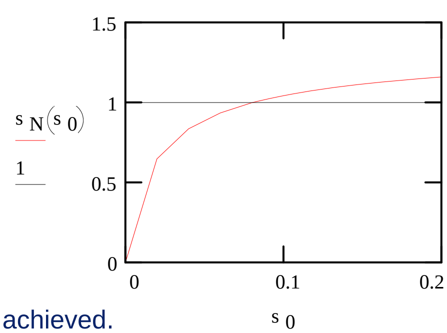
Add one point to separate lines. $s_{j,N+1} := 999$ $\quad r_{N+1!} := 999$ $\quad i := 1 .. N+1$



It is obvious that a different initial value of s at r=0 leads to a different value of s at r=1.

The value of s_N at r=1 is a function of the initial condition (s at r=0, or s_0). $\quad s_0 := 0, 0.02 .. 0.2$

$$s_N(s_0) := rkfixed\left[\begin{pmatrix} s_0 \\ 0 \end{pmatrix}, 0, 1, N, ODE\right]_{N,2}$$



$s_N(0.0805) = 1$ ← manually guess s_0 until s_N=1 is achieved.

Find s_0 with the "root" function. With the last function definition, we can let the computer find the correct initial condition.

$s_0 := 0.5$ ... initial guess

$s_0 := \mathrm{root}\left(s_N\left(s_0\right) - 1, s_0\right)$ $s_0 = 0.0805$ ... the correct initial condition

Find s_0 with the "Given-Find" function.

$s_0 := 0.5$ ... initial guess

Given $s_N\left(s_0\right) = 1$ $s_0 := \mathrm{Find}\left(s_0\right)$ $s_0 = 0.08055$ ... the correct initial condition

Once we find the correct initial condition, integrate the ode once more to find the solution to the boundary value problem.